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Lec 14: Analysis and Engineering of 2D Photonic Band Structure

Hello students, welcome to lecture 14 of the online courses on Photonic Crystals Fundamentals and Applications. Today's lecture will be on analysis and engineering of 2D photonic band structures.

Lecture Outline

- **The Physical Origin of Photonic Band Gaps**
 - **Meaning of Photonic Band Gap (PBG)**
 - **Fabrication of PBGs**
 - **Working mechanism of PBGs**
 - **Physics of PBG**
 - **Formation of PBG**
- **Band Structure Analysis of 2D Photonic Crystals**
 - **Simulation of the Band Diagram**

So, today we will be discussing the physical origin of photonic band gaps. that will cover the meaning of photonic band gap, how do we fabricate those structures and how do you get the band gap. We will discuss about the working mechanism of photonic band gaps, the physics behind it, formation and then we will take up an example of 2D photonic crystal and do the band structure analysis using a video. will show you the simulation of a band diagram using COMSOL multiphysics.



The Physical Origin of Photonic Band Gaps

The Physical Origin of Photonic Band Gaps

What is a Photonic Band Gap ?

- A photonic band gap (PBG) crystal is a structure that could manipulate beams of light in the same way semiconductors control electric currents.
- A semiconductor cannot support electrons of energy lying in the electronic band gap.
- Similarly, a photonic crystal cannot support photons lying in the photonic band gap.
- By preventing or allowing light to propagate through a crystal, light processing can be done

Okay, so let us first discuss about the physical origin of photonic bandgaps. So, a photonic bandgap crystal is basically a structure that can manipulate beams of light in the same way electrons could or you can say the semiconductors could control the flow of electrons or the electric current. A semiconductor can support, a semiconductor cannot support electrons of energy that lies within the electronic band gap and similarly a photonic crystal also cannot support photons which has got energy lying within the photonic band gap. By preventing or allowing light you know based on its energy to propagate through the crystal or getting reflected you know you can do light processing.

The Physical Origin of Photonic Band Gaps

How is a PBG fabricated ?

- Photonic crystals usually consist of dielectric materials, that is, materials that serve as electrical insulators or in which an electromagnetic field can be propagated with low loss.
- Holes (of the order of the relevant wavelength) are drilled into the dielectric in a lattice like structure and repeated identically and at regular intervals
- If built precisely enough, the resulting holey crystal will have what is known as a photonic band gap, a range of frequencies within which a specific wavelength of light is blocked

And that is where you know photonic band gap crystals are used for. So, how is it fabricated? So, as you already know that photonic crystals usually consist of dielectric materials, okay. That is materials that can serve as electrical insulators or in which you know an electromagnetic field can propagate with minimal loss. holes which are of the order of wavelength can be drilled into a dielectric medium in a lattice kind of structure and it can be repeated periodically at regular intervals and that can give you a crystal. So if you build that precisely, the resulting crystal will have what is called as the photonic band gap.

That means it will have a range of frequencies or wavelength which will be blocked from entering into that particular crystal.

The Physical Origin of Photonic Band Gaps

How does a PBG work ?

- In semiconductors, electrons get scattered by the row of atoms in the lattice separated by a few nanometers and consequently an electronic band gap is formed
- The resulting band structure can be modified by doping
- In a photonic crystal, perforations are analogous to atoms in the semiconductor
- Light entering the perforated material will reflect and refract off interfaces between glass and air .
- The complex pattern of overlapping beams will lead to cancellation of a band of wavelengths in all directions leading to prevention of propagation of this band into the crystal .
- The resulting photonic band structure can be modified by filling in some holes or creating defects in the otherwise perfectly periodic system

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Source: <http://optoelectronics.eecs.berkeley.edu/ey1993josab102.pdf>

So how does it work? As I mentioned in semiconductors electrons get scattered by the row of atoms in the lattice which are separated by a few nanometers and consequently a electronic band gap is formed. ok and the resulting band structure can be modified by doping in the semiconductors right. In a photonic crystal perforation or the holes which are drilled ok these are basically analogous to the atoms that is in the semiconductor right. So, here when light enters a perforated material that will get reflected and refracted from the interface between glass and air.

Whereas air that is basically the hole right. So, you have usually these are made on silica material or silica slab. So, that is why you know glass is mentioned okay. So, a complex pattern of overlapping beams could actually lead to cancellation of a particular band in all directions. which tells you that that particular you know wavelength is not allowed to propagate through the crystal and that is how you get your band gap.

So the resulting photonic band structure can be modified by filling some of those holes or by creating defects like making a smaller hole or a larger hole, which is otherwise a very perfectly periodic system.

The Physical Origin of Photonic Band Gaps

Physics of PBG

- In the 19th century, Maxwell's theory of electromagnetism, later verified by Hertz, laid the foundation for wireless communication, evolving into modern radio, TV, and mobile phone use. Recent discoveries reveal light waves can be trapped, not just propagated.
- Trapping and micro-molding light require materials with stronger light scattering than natural ones.
- Multiple light scattering occurs on cloudy days, with sunlight scattering from water droplets in a cloud.
- The mean free path is the distance light travels in the cloud before scattering randomly.
- Light transmission through a cloud is reduced based on the cloud thickness to mean free path ratio, with scattered light making clouds appear white.
- The invention of the laser revolutionized light technology, enabling precise probing of matter, advanced medical tools, and high-speed data transmission via fiber optic cables, allowing clear global communication.

So in the 19th century, Maxwell's theory of electromagnetism, which was later verified by Hertz, that laid the foundation for wireless communication that involves modern radio, TV, telephone, and mobile phone, mainly mobile phone. We're talking about the wireless communication. Recent discoveries reveal that light waves can also be trapped, not just propagated. Trapping and micro-molding light require materials with stronger light-matter interactions and stronger light scattering than the natural ones.

Multiple light scattering occurs on cloudy days that we can see with sunlight getting scattered from the water droplets in a cloud. The mean free path is the distance light travels in the cloud before getting scattered randomly. When you talk about light transmission through a cloud, it basically gets reduced based on the cloud thickness to mean free path ratio. That actually tells you why the clouds appear white. It's because of the multiple scattering.

Now, with the invention of the laser that actually revolutionized light technology that allows precise probing of matter. So, you know, you can actually use it for advanced medical tools, high speed data transmission, something like fiber optic cables, which allows global communication. But with all of these, what is important is that Clouds or human tissue, they scatter light strongly enough to localize it. So when you say localization, localization requires microscopic dielectric structures that could scatter light a thousand times more strongly than human tissue. So this results in a transport mean free path which is as short as the length of the light's wavelength.

The Physical Origin of Photonic Band Gaps

Physics of PBG

- Clouds and human tissue cannot scatter light strongly enough to localize it.
- Localization requires microscopic dielectric structures that scatter light a thousand times more strongly than human tissue.
- This results in a transport mean free path as short as the light's wavelength.
- A periodic arrangement of these scatterers can remove light propagation pathways over specific frequency intervals.
- Complete removal of light propagation pathways over a band of frequencies in all directions creates a photonic band gap (PBG).
- Dielectric microstructures that exhibit this effect are known as PBG materials.

So, a periodic arrangement of this kind of scatterers can basically remove light propagation pathways over specific you know frequency interval and that is the physics behind the photonic band gap. So, complete removal of light propagation pathways over a band of frequencies in all directions could create the photonic band gap PBG. So, dielectric microstructures that exhibit this kind of effect are known as PBG materials

The Physical Origin of Photonic Band Gaps

Physics of PBG

- In electronic micro-circuits, thin metal wires guide electrical currents, with electrons confined by the metal's work function.
- Optical waves differ; though optical fibers guide light, micro-circuits of light based on fibers are not feasible due to light escaping into the background.
- Empty space is an ideal conductor of light waves, allowing light in optical fibers to escape if the fiber is bent or distorted microscopically.
- PBG materials solve this issue by eliminating all background electromagnetic modes over specific frequency bands.
- Light paths can be engineered within PBG materials as waveguide channels, localizing the light and preventing it from escaping the optical micro-circuit.

In electronic microcircuits thin metal wires guide electrical currents ok, where basically the electrons are confined by the metals work function and if you think of optical wave they differ. though optical fibers guide light micro circuits of light based on fibers are not feasible because light could escape

into the background.

So, empty space is basically an ideal conductor for light waves which allows light in optical fiber to escape okay. So, fiber if it is band or distorted microscopically there is leakage. So, PBG materials could solve this issue by eliminating all background electromagnetic modes over specific frequency bands and that is why when you have photonic band gap crystal being used for very sharp bands there is no leakage. So, you can actually guide light over very sharp bands in micrometer or micrometer scale. so light paths can be engineered within pbg materials as waveguide channels localizing the light and preventing it from escaping the optical micro circuit okay

The Physical Origin of Photonic Band Gaps

Physics of PBG

$\epsilon(x) = \epsilon_0 + \epsilon_{\text{fluct}}(x) \longrightarrow \text{Eqn (A)}$

Here, ϵ_0 is the average part of the dielectric constant and $\epsilon_{\text{fluct}}(x)$ represents the part of the dielectric constant that varies from point to point in space.

- The wave equation for such an optical field is given by:

$$-\nabla^2 \vec{E} + \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) - \frac{\omega^2}{c^2} \epsilon_{\text{fluct}}(x) \vec{E} = \frac{\omega^2}{c^2} \epsilon_0 \vec{E} \longrightarrow \text{Eqn (B)}$$

Analogue of the "kinetic energy" terms in Schrödinger's equation
 Plays the role of scattering potential
 Analogous to Energy eigen value

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 Source: <https://www.physics.utoronto.ca/~john/john/Encyclopedia.pdf>

so now let's look into more fundamentals of how exactly the photonic band gap is created so the The question of whether light can be localized okay can be posed in the form of an analogy between Maxwell's equation for electromagnetic waves propagation and Schrodinger's wave or Schrodinger's equation for electron propagation.

let us consider a monochromatic electromagnetic wave of frequency omega propagating in a medium whose dielectric constant varies from a point to a point in space which is given by this particular equation. So, you know there is a fluctuation in the dielectric constant which is given like this. So, we assume that the dielectric microstructure does not absorb the light and the total dielectric constant everywhere is real and positive. So, in that case you know the wave equation for such an optical field can be given by this equation which is equation B okay and this can be written in a form which resembles the quantum mechanical Schrodinger's equation right. So, here the first two terms that you see are analogous to the kinetic energy terms in Schrodinger's equation.

okay unlike electrons which can be trapped and localized for negative eigenvalues okay So here you

can see that this term is analogous to the energy eigenvalue and this fluctuation term okay, this plays the role of the scattering potential right. So unlike electrons which can be trapped and localized for negative eigenvalues which are bound states in corresponding negative energy potential wells. the overall positivity of the dielectric constant in this particular equation leads to the constraint that the energy eigenvalue is always greater than the highest of the potential barriers presented by the scattering potential. So, with that you can think of the formation of photonic bandgap

The Physical Origin of Photonic Band Gaps

Formation of PBG

- Photonic band gap formation can be understood as a synergetic interplay between two distinct resonance scattering mechanisms.
- One is: The microscopic scattering resonance from the dielectric material contained in a single unit cell of the photonic crystal.
- Second is: The macroscopic resonance from the geometrical arrangement of the repeating unit cells of the dielectric microstructure.

Figure: Photonic Band gap formation

So the photonic bandgap formation can be understood as a synergetic interplay between two distinct resonance scattering mechanism.

So what are those? The first one is the microscopic scattering resonance from the dielectric material contained in a unit cell of the photonic crystal. So here you can see you can consider a periodic variation of permittivity. So, this is the lattice constant L okay and you can think of this is done by some kind of sphere air-air sphere which is drilled and you can take why I call this is air because this is the lower refractive index and this is the higher refractive index. So, this radius can be marked as A okay. Now this actually shows the scattering of a wave by a square well potential.

When you can see here when half of the optical wavelength fits into the width of the well that is the case where transmission from left to right is maximum and least amount of light is reflected. But when one quarter of the wavelength fits into this well width that time least amount of light is transmitted and the maximum amount of light is reflected. So, maximum you know reflection happens when you know $\lambda/4 = 2a$. This is the width of the well is $2a$ and that is equal to $\lambda/4$. So, that way you can also find out that what is the condition for maximum reflection.

So, this is for individual. So, one resonance is for the single unit cell and then there is another type of resonance which is the macroscopic resonance from the geometrical arrangement of the repeating unit cells of the dielectric microstructure. So, that is basically now telling you about the

other resonance. So, if there is a periodic arrangement of unit cell which is there in the photonic crystal, you can call this kind of scattering as Bragg scattering. So, this occurs when the spacing between the unit cells which is basically the lattice constant L is basically an integer multiple of λ by 2.

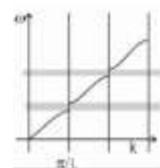
So here you can see that is the case when the resonance happens and maximum reflection takes place. So if you see this k vector okay, so at integral multiple of π by L okay, there is this kind of reflection that means bandgap formation taking place. So, what you understood that band gap formation is basically facilitated if the geometrical parameters of the photonic crystal are chosen such that both microscopic that is within one unit cell what is happening that resonance and what the overall periodic structure that is the Bragg scattering resonance that is the macroscopic resonance both can coincide at the same wavelength and that is where you will be able to see the photonic bandgap formation okay. So, here is the dispersion relation which is ω k diagram in case of photon in vacuum. So, you can see a straight line in the case of photon in a periodic dielectric medium you can see that the relation more or less you know follows that similar pattern but there are discontinuities at integral multiple of π by L okay.

The Physical Origin of Photonic Band Gaps

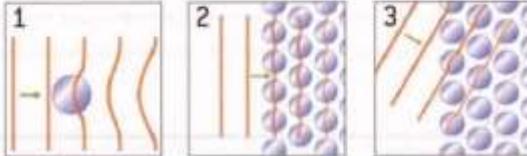
Photon in vacuum



Photon in periodic dielectric



Wavelength in a 2D PBG



- For a two dimensional band gap, each unit cell of the structure produces reflected waves.
- Reflected and refracted waves combine to cancel out the incoming wave.
- This should happen in all possible directions for a full 2D bandgap.


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Source: <https://empossible.net/wp-content/uploads/2025/05/Lecture-Electromagnetic-Waves-in-Periodic-Structures.pdf>

So, we have also understood that this kind of alternative dielectric structures when they are having high contrast that can give rise to wider band gap and the band gap size can thus be changed. This is how you know what happens in a 2D photonic band gap. So you can think of a single scatterer which can you know this is a dielectric material. So when a plane wave falls on that the part of the plane wave which is going through this material slows down because the speed of light in this material will be reduced by a factor of n which is the refractive index of this material as compared to the vacuum speed of light okay or you can say speed of light in vacuum okay. So, that way you can see that if you have a periodic modulation like this the amplitude of the wave will also get modulated but then every unit cell produces some reflected wave okay and when the reflected and the refracted wave

they can combine and cancel out the incoming wave you can say that there is photonic band gap and that has to happen in all possible direction to give you a complete photonic band gap.

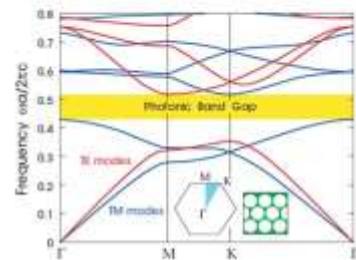
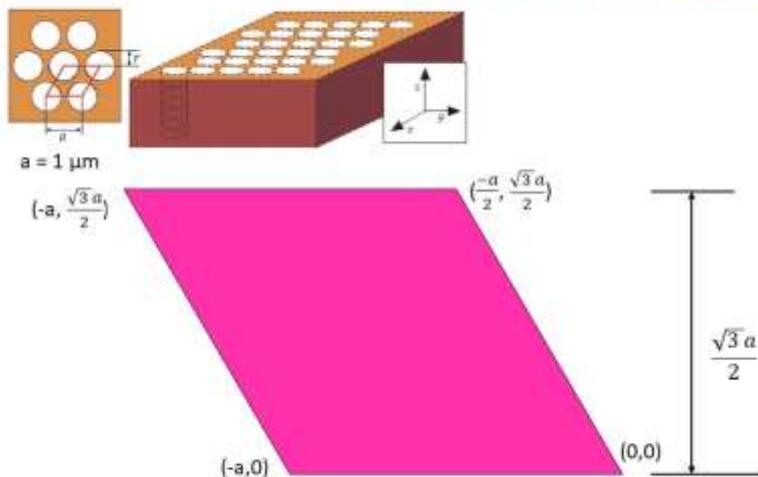


Band structure analysis of 2D Photonic Crystal



Now let us go into the analysis of band structure for a 2D photonic crystal. So, now here we will see how to simulate the band diagram for a 2D photonic crystal in a commercially available FEM software that is finite element method software COMSOL. We will not go into more details of COMSOL we will just show you an example how to do it. ok. You can do it using other methods as well ok.

Simulation of the Band diagram



Source: Joannopoulos, John D., et al. "Molding the flow of light." *Princeton, NJ [ua] 12* (2008).



This is popularly used for calculating bandgap. So, we are showing some example here ok. And we will take this particular example from the book which is from the chapter 5 of this particular book okay. So, there is a video coming in the after this slide that will explain you know all the physics and how to simulate this structure. So, what is this structure as you can see this is basically a hexagonal array of holes being drilled in a particular dielectric medium.

So, this is the rhombus that is shown here ok. So, these are the coordinates marked $(0, 0)$ minus a_0 minus you know $\frac{3}{2}a_0$ comma $\frac{\sqrt{3}}{2}a_0$ this point and this point is this one ok. So, I think in the video there is a typo here. So, just take this as the correct one in the video there is a typo. So, ignore that and we will show you how to get this kind of a band gap.

So, now we will show you a video that show you the method of calculating all these things and generating this photonic band diagram in COMSOL. So, this is done by Dibaskar Biswas who is the TA for this course.

Simulation of the Band diagram

Real space vectors

$$\vec{a}_1 = a_0 \vec{a}_x$$

$$\vec{a}_2 = a_0 \left(\frac{1}{2} \vec{a}_x + \frac{\sqrt{3}}{2} \vec{a}_y \right)$$

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Okay. So hello students. So in this video, we'll see that how we can simulate the photonic band diagram of a 2D photonic crystals.

So here I have taken this actually a structure from the book called the molding the flow of light. So you can see that this is a kind of structure. So this box actually, the rectangular 3D box, it is a dielectric box. And inside this box, circular holes have been drilled. So you can see that this is a kind of a lattice structure.

And this is actually repeated along the entire rectangular box. And so you can so we shall simulate this band diagram, as you can see here for both the T modes and TM modes and in the software commercially available that is Comsol. So before that, we shall quickly go through the basics and basic theory of it, that how we can calculate the band diagram. So we need to see that. So, first of

all, we see that this is a circular, like this is a hexagonal shaped lattice.



And so, and also we can derive the rhombus lattice also by taking the midpoint of all the circles. So, the center of all the circles, joining all the centers, we get the rhombus unit cell. And the A is the lattice periodicity or lattice constant. Or we can say that the length of the rhombus is given by the lattice constant extra leap. so we shall work on the rhombus unit cell in COMSOL so as you have seen from the from lecture 9 actually that for a hexagonal lattice or rhombus lattice the in real space in reciprocal space we get the hexagonal we get a hexagonal Brillouin zone For a square lattice, we get a triangular Brillouin zone.

First of all, for simulating the band structure in COMSOL, we need to see how a rhombus actually is drawn. For a rhombus, we need to first know the coordinates of it. So, the height of the rhombus actually it is given by the $\sqrt{3}a/2$ and the coordinates are actually here the $0, 0$ this is the $0, 0$ minus $\sqrt{3}a/2$ and $a/2$ and $a/2$ because this will come as a midpoint length. But here actually we are simulating the band structure in a 2D platform. So we are concerned only with A_1 and A_2 vectors.

So A_3 will be taken as a constant here. So as we take the A_3 vector as a constant number, so it gets cancelled out. So, from there B_1 can be calculated as this that is $\sqrt{3}a/2 A_x - a/2 A_y$ and B_2 is $a/2 A_y$. So, here $\sqrt{3}a/2$ is nothing but a number actually. So, in order to simplify the our formula the expression for B_1 and B_2 we have written cannot as this 4π by $\sqrt{3}a$ naught. now after calculating the the reciprocal space vectors now we need to we shall go for the irreducible Brillouin zone that is here so you can see that this is the Brillouin zone and this is the irreducible Brillouin zone see if we replicate this Brillouin zone here this another triangle then this will be another Brillouin zone This will be another Brillouin zone.

See if we replicate go on replicating this we get actually the entire Brillouin zone. So that's why it is called the irreducible because we can't reduce it further. So this is the shortest or the optimized zone actually. So, here the center of the Brillouin zone is given by the τ point.

Tau mk are the actually high symmetry points. So, the origin of the Brillouin zone is given by the tau point. The midpoint of one of the edges of the Brillouin zone is given by the m point and one of the corners is given by the k point. So, we need to know the coordinates because we will be taking k vector. So, this k vector will sweep from this entire irreducible Brillouin zone. so it will come back again from it will start from tau and it will go from tau k m then again it will come to tau as you can see here in the band diagram also the k vector so this is the uh this axis is the k vector and this is this y y axis is the eigen frequency that's how we get the band diagram so this k vector sweeps from tau point c to m then m to k then k2 again tau uh so we need to know the coordinates first here so how you can see that we have already calculated here the k vector is given by $\frac{2}{3} b_1 + \frac{1}{3} b_2$ so how we have calculated here is that so as you can see that this is the k point And this is the endpoint.

OK, so we need to go from the origin that is the tau tau here to K this, but we can't go directly from tau to K in in this line. So for that we need to move along the vectors. So the only vector which we can see that the easiest path is the is along B1. So along B1 we move from starting from the origin. so we go up to here and then we move from here to this point So now what is the total length? So you can see that this is actually $\frac{2}{3}$ of B1.

Like if we cut B1 into three components, so we get this length as this length as $\frac{2}{3}$ of B1 and this straight length. If we again cut B2 into three components, so this length will be equal to this this path. So that is nothing but $\frac{2}{3}$ of B1 and $\frac{1}{3}$ of B2. So that's how we get the K point.

So this is the coordinate $\frac{2}{3}, \frac{1}{3}$. So tau is actually simple because it is in the origin. So we are not moving along b_1 and b_2 . So it is $0, \frac{1}{3}, 0, \frac{2}{3}$. That is $0, 0$.

And for m actually, what we do is that, let me rub it. So let me draw again this part. Okay, so for M, we actually again move from this direction and we go to this edge. That is the midpoint of the edges of one of the edges of Brillouin zone. So we go here, then we go from there to this point to get the M point. so this is nothing but half of b_1 and this length this horizontal line is nothing but half of b_2 so that's how we get the m point so we got we got all the coordinates for that is for tau of high symmetry point that is tau km now we define uh this k vector so this is important because we will be sweeping sweeping this k vector uh to get this uh this axis axis values okay So, k vector is nothing but αb_1 .

So, αb_1 is nothing but it is written here as an expression it is actually the b_1 vector only. So, αb_1 vector plus βb_2 vector. so we'll put this b_1 expression here and b_2 expression here and we'll reorganize the components to get actually k vector in terms of so one component will come like this like this if i write k vector like this so one component will come as x and another component some expression will come as a y So this actually is your KX component and this actually is your KY component. So this two terms are important because we will be using this in our console simulation.

So. Alpha now the question is what are what is alpha and beta alpha and beta are nothing but two numbers actually. So these are basically some equations will be under some definite conditions. so what are the conditions actually we will see in the next slide so we require the conditions for alpha

and beta and that will be used in the console so we define actually a k it is here it is a magnitude here so k is swept from tau to you can see tau to m then again m to k then k to tau So, we designate tau as the origin as 0, m as 1 and k as 2 and tau as again 3. So, do not get confused with the coordinates actually because these are the vectorial coordinates and these are actually the designated numbers that is this is not a vector, this is a scalar quantity and it is being swept from 0 to 3 and this is a vector notation.

So, these two are different. so after giving the notation the from 0 to 3 so now we can actually calculate this alpha and beta So the alpha and beta are given by these conditions like from 0 to 1 the alpha is given by this condition 1 to 2 alpha is given by this and 2 to 3 alpha and given by this similarly it is same for beta also. Now how we are getting this expression these are actually purely intuitive based there are no specific or definite formulas are there from where we have calculated it. You just need to check the these coordinates 2 by 3 1 by 3 because we are moving from C tau to M.

So we are moving from 0 to 0 comma 0 to 0.5 comma 0.5. then 0.5 to 2 by 3 we are going so you need to put in alpha and beta you need to write equations in terms of k so that for this range c is for this so there are three ranges 0 to 1 1 to 2 and then 2 to 3 so for each of the ranges you have to put you have to write some equations that will satisfy these coordinates actually so if i like put one here so uh that will be calculated alpha will be calculated as $0.5 k$ that is k by that is k by two so for k equals to one k equals to one means the m point this is the m point so for m point you see this is the 0.5 okay that is your half of b_1 so that is your k by 2 actually so for k equals to if i put k equals to 1 we get alpha equals to half and that is nothing but your alpha this value half of b_1 because we're writing k vector as alpha b_1 okay so b_1 is this and alpha is your half so you need to write those expressions intuitively such that this satisfies if you put whatever value here in the expression for alpha and beta you get this vector notation again okay so after achieving these expressions for alpha and beta we'll we'll use this condition and also this sweeping of k vector we'll also use these conditions here So this is the design methodology how we will actually like this is the actually design you can see this is the rhombus rhombus unit cell and you can see that some part of the circle is inside the unit cell actually. So how we will design it actually so first we shall design the rhombus here in comsol using the coordinates and then we shall draw circles Whose radius is actually at the at one of the endpoints of the rhombus and then we shall remove this part so so that this section of the circle remains inside only this section remains inside the circle.

OK, so the basic theory is I think it is clear. So now we shall move to the console interface. So whenever you open.

OK, let me. Close this. Let me open console again. Whenever you open console like this, it will take one minute time and then you will get an interface. You will see it soon. In this interface, this will open up in your laptop or desktop. You can see that there are some number of options called file, home, geometry, material.

These will be discussed later. Here, this is the important part that is your model wizard and blank model. So blank model is nothing but these are used by the developers actually where they have the freedom. Blank model means that you have the complete freedom to include whatever kind of physics or module you want. And model wizard is like by default you have to select physics and then

the module actually and by default they will give some parameters like global parameters then whatever the geometry part the components they will come by default but in blank model nothing will come by default you can add it so that is the freedom so before going to that let me give a brief overview about comsol comsol is nothing but it is a multi physics simulation software Multiphysics means like you can put multiple kind of physics like the for solving any kind of thing you can like implement multiple physics to solve a complex structure how the structure is behaving. So, it is actually used for modeling and simulating the physics-based problems that is widely used in engineering physics and applied mathematics to simulate the behavior of systems in various fields.

These fields are like electromagnetics where this is used for designing and analyzing the electromagnetic devices. wave propagation and electromagnetic modes. Then structural mechanics, they are acoustics, fluid flow, heat transfer, chemical reactions. These are all the applications where the COMSOL is used. You then click here, Model Wizard, then for band diagram it as it is a 2d diagram so 2d band diagram so we are the geometry is also in 2d so we will click here 2d and there you will see that a pop window will pop up that is you need to select the physics so you go to this radio frequency click here and then you shall see that electromagnetics frequency domain so that is the emw so you click select this then you add After this will come here then after adding this you need to go to the study.

So what what you need to study here because you have selected the physics. Now what kind of what is the thing you want to study whether it is the mode what is the whether it is the time domain analysis of frequency domain or or eigen modes. so you click here so you see that in the top it is given as eigen frequency so you click here and then you hit done so after that comsol will take you to the main interface you can see this is the model builder window see by default it has come global definition component definitions and mesh size study results okay so we shall discuss one by one So this is the interface where your geometry will be seen and after coming to this interface you have to first what is the first work is you have to define the length unit. So as you have seen here our lattice constant is in micrometer. So we shall define okay we shall take the geometry as micrometer here and then we shall go to global definition that is the parameter and we shall define all the parameters here that is the lattice constant then k vector not k vector that is the scalar k then the k_x and k_y and the radius of the circle we shall define one by one so i have already simulated the structure here so because that will take a lot of time for designing and then simulating so these you can see here this is the parameter this is the lattice constant you write one then third bracket then for micrometer not u is the symbol for micro so you write it like this and comsol will take the value see 10 to the 1 minus 6 then you define alpha and beta so see here comsol actually takes this kind of equations as by condition called if and else condition So, how it works actually we see if k lies between 0 to 1 then alpha is 0.5 k else if k lies between 1 to 2 then alpha is this else if k lies between 2 to 3 then alpha is given by this.

So, how do we write it like this? in console so he like we write if then give first bracket okay then write not 0 less than k less than 1 we just write k less than 1 only k less than 1 then comma alpha value is 0.5 into k then comma else if we do not write else we write just only if so if then again we start the bracket then we write k less than 2 if for k less than 2 alpha is 1 by 6 into k plus 2 then we give comma then we don't write l else we just write the final value that then there is the third value for 2 to kl for the range of 2 to 3 we write alpha is 2 by 3 into 3 minus k then we close the bracket

for the first if and then we close the bracket for the that the final if so if you don't close the bracket no if you give incomplete bracket then comsol will give an error see fail to evaluate expression for parameter alpha so it should be careful about the closing of brackets So, same it is done for beta and then we take this scalar k, we initialize it, we give some value, it can be like 0, it can be like 5, 7, whatever value is it, we just, you just need to initialize it, okay. So, this k actually will sweep from 0 to 3. So, as you have seen here, this is the k, this is the k actually here.

So, this will sweep from 0 to 3. So, we have initialized it okay and then $k \neq 4\pi$ by $\sqrt{3a}$ as you have seen in the expression for b_1 and b_2 k_x and k_y so k_x and k_y is actually αk_x is α into k not $\sqrt{3}$ by 2 and k_y is this by given by this expression r is the radius it is taken from the book actually now after doing all this we go to the geometry part So for rhombus actually what we do is that we write all the coordinates here. We take for rhombus actually like you click the geometry here and then you go see there are no rhombus options is there. So you need to click polygon. So after clicking polygon you just rename the level as rhombus and then you go to the table here and you give all the coordinates whatever coordinates for the rhombus it is given and then you hit build selected you see your rhombuses will be visible in this screen design screen.

Now you go for the circle. The geometry it is pretty much simple circle is there. You just go there, give the radius and the circle center. The center is actually I told that one of the four endpoints of rhombus. So first endpoint is the origin here.

So this will be 00. So you click build selected. So now you see the design is not entirely visible in the screen. So you go there and that is the zoom extends. You click here. So now the design is visible completely. for circle two same minus a comma zero this then circle three then circle four so you uh hit again click here zoom extends now the design is visible now you see that uh we don't require this part of circle so we need to uh remove this part of the circle so what we do is that we go geometry and then booleans and partitions is there we click here and then we go for partition domain so this option will come let me remove this now we need to what is the domain so domain means a structure okay this is the structure circle so these are all domains so we need to partition this domain into this segment and and this sector sector segment okay so we need to click this this this four circle we need to domain and partition with okay so partition with what so we need to partition with this edge so this two edge will separate this circle into two components so we need to click here edges and then we click this edge this edge this and this okay then we click build selected okay so now our domains have been partitioned now we go again to the geometry and then we click here this delete option we come here and then we select called the domains by default it will be in object so you click here domain and then you go there see now the domains have been separated see so you click this this this and this so now you click build selected and then you click build all objects okay so you see that now our design has been is ready okay now you need to put the material because this four sectors of circle will be filled with air and this and this part that is the this shape will be filled with dielectric so for this you go to material option then you click add material so this add material interface will come here so here you go see this is the built-in option you click here then you click air and then you click add to component after clicking not to global materials but add to component so here under the component option this material part air will come okay So this is the air and for dielectric you again go to add material and then you again click air this this will come and then you rename it as dielectric actually.

So after that you need to give the relative index of the dielectric. So for that you go to this electromagnetic wave that is the physics interface and you it will be like this actually in console you expand it and then you go to wave equation. There you go down and you see that electric displacement field. So, your electric field or your magnetic field whatever you are visualizing. So, that is actually by default console here you will get this option relative permittivity.

So, you change it to refractive index. and then you go again to air then you go to material contents and then you give this option will you will see two tick marks for refer to index real part in imaginary imaginary is zero so for dielectric you give a square root of 13 because if it is given by root over of the dielectric constant and this value is actually taken from the book itself so you will get this value so square root of 13 and for one air it is actually one okay so now we all these materials have been defined uh we go to the periodic condition so for periodic condition you click here now you select this and then you right click here so you will see that this is the periodic condition you click here so this option will come now you have to select the boundary because here it will come uh manual okay you select manual and then you give the periodic condition now you see that this entire rhombus lattice is actually repeating infinitely in the x direction and also in the y direction okay so that's how we get a 2d photonic crystal because this is the basic definition 2d photonic crystal means the lattice is repeating in two two dimensions okay so as you can see that this lattice is repeating in x direction and y direction also so that's how we get a 2d photonic crystal so here you select this face and carefully select it okay so you select this also so how i have moved this structure you just right click on the mouse and then click it and then drag it okay so then you select this select this and select this also this because these two sides becomes a constitute a pair of a periodic face okay so these two sides you have to calculate it like this is one side you select all the boundary and this is one side selected boundary this is the first periodic condition now for second periodic this is this face and this face so for second periodic you click you go there click again periodic condition and this will come okay then you select all the boundaries this boundary this and then opposite face this three boundaries okay now uh after giving uh you need to go down to the periodic condition here you will see type of periodicity so you have to select the floquet periodicity and under floquet periodicity you have to define the k vector so here you have to define k_x and k_y okay for both periodic condition 1 and periodic condition 2 so after doing this you go to mesh so what is mesh actually now see we have all studied the Maxwell equations how the Maxwell equations are solved but all these theoretical analysis that you have done for Maxwell's equation these are actually for infinite kind of structures or boundless structures but in reality in reality actually all the structures are finite that is bound okay so for finite structures the Maxwell equations actually like changes a bit so what the software does is that it will divide your entire rhombus whatever structure is there it will divide your structure into very minute geometric shapes okay it can be triangle it can be tetrahedral okay depending on the availability of structures in in the software so it will be divided into small small geometrical shapes and there the console will for each geometrical shape console will solve the the Maxwell equations and whatever values it will it will achieve it will store it in the matrix okay so this is the kind this is the definition of actually mesh so you have user control mesh and physics control mesh physics control mesh is that the meshing is controlled by the physics that you have selected that is the electromagnetic wave frequency okay and another one is the user control user control means you have the control to like you have the freedom to like to simulate your structure like if suppose say this sector of a circle is very small the like say suppose it is coming here it is this the size

is very small so physics control mesh won't be able to take won't be able to divide that small structure into very fine geometrical shapes so there you have to select the user control mesh and then have to uh go for a very fine mesh there okay so you have that freedom but in physics control mesh like the in this structure we don't require uh that kind that much kind of finer mesh so you just click physics control mesh then you see element size element size that is the what is the size of the smallest geometrical element of the mesh okay so there are a number of options from extremely coarse to extremely fine so we just we are taking the finer option because if we go higher also so that will take a huge amount of computation time and also it depends on the availability of ram so if your ram is like less than 8 gb that is 4 gb then it might create a problem simulating the structures with finer mesh So, with 8 GB RAM or 16 GB RAM, we can easily handle this. So, we are taking finer mesh and then we are clicking build all. So, see these are the small, small, small triangle structures. So, that is dividing actually. So, console will solve the Maxwell equations for each of this triangle and then it will save it, save the data into the matrix.

so after doing all this we go to study so here in the study you will see this parametric sweep option won't be there okay so let me delete it i will tell you again so in uh this option will come eigen frequency so here you go to this option called desired number of eigen frequencies so see here and how many bands are there for t mode one two, three, four. Okay, four bands. So I have taken here actually six bands. So number of, you can take four also, you can take six, but don't take much because it will increase the computation time. And this is the unit, unit is in gigahertz I have taken, or you can take it actually in terahertz also, but that doesn't matter, that will not hamper your simulation.

but this is the important search for eigen frequencies around so you take write it as one here and in bracket third bracket give it as as terahertz why terahertz because like the lattice constant diameter you can see that it is in micrometer one micrometer so the eigen frequencies will be coming in the terahertz actually frequency range okay because if you do the c by a analysis so that will be in the 10 to the power 14 dimension okay so the range actually so it will be coming in the one terahertz and then again frequency search method around shift you keep larger real part because in if you click here closest absolute value then they don't give the result it will give a wrong result so you keep larger real part here and then you go to study one again click here right click then you go to parametric sweep so as i have told you that k that scalar quantity it sweeps from zero to three so you click all combinations here then you click plus here see the parameters whatever whatever we have defined it will come here so you click here k then you go to click this parameter value list and this is the option called range you give the range here so entry method is step number of values logarithmic okay so you give number of values here so it starts from zero but we don't start it from zero because at the zero and at three there are actually discontinuities okay so we don't want those discontinuities so we just avoid this we click 0.1 and it stops at 2.9 and number of values that is the interval so it you can take it depending upon the like resolution for higher resolution bands you can take higher number of values but here for getting the simulation in lesser amount of time we take 52 or 55 maybe that is greater than 50 okay when you click replace or add and then okay after doing all this you go to home then build all then again build mesh and then you click compute OK, so here you see the solver actually will the has started the assimilating, so it will take a few minutes one in one or two minutes.

It will simulate the structure. You can also in the progress button. You can also see the how the progress is going on. That is 76 78%. OK, so it is almost done. okay so after getting this plot you can see this is the electric field normalized electric field plot so if you want to see the magnetic field you just go there in the results option you will see electric field emw click expand this go to surface then here data set will be your parametric solution solution to okay you click this Then you see this is the expression you see parameter value k is there all the parameter values have come and the all the eigen frequencies are there. So, this is the emw dot norm e that is a normal electric field you just remove this only emw dot you just keep there and you keep h z just click there and see.

So, this is the your this is the t mode. So, there is the z component of magnetic field. along the your entire the your 2d lattice unit cell structure now for getting the band diagram you click on the results and then right click you go to 1d plot then you click this parametric solutions okay you come again to 1d plot group 2 you click this right click again you go to global option There you click parametric solution to here. Now you have to define the Y axis. Now Y axis is your eigen frequency, so you have to click EMW OK dot FR EQ OK into a. divided by that is your the velocity of light that is the c so c is actually by default comsol takes the name of c underscore constant so this is the and you click there enter this will come and this expression is nothing but your uh this uh this one ωa by $2\pi c$ so ω if you expand it $2\pi f$ so your 2π 2π get cancelled so it is actually f into a by c so i have done actually this one okay so f into a by c so this is the y-axis data for x-axis you just change it from eigen frequency to outer solutions and then you go to this plot option click here It will take few seconds.

See. So, we have got the band diagram. Okay. So, this is your band diagram for the TE mode. So, for this is the kind of this is the legend actually called. So, you can remove it by going to 1D plot group again. and go down and click off so you see this for the TE mode so see the t mode this is one band and then we get a photonic band gap and then again the band start so yes see this is the first band first eigen frequency band then we get a photonic band gap and then the band gap starts so this is for the TE mode now i won't like simulate again for the tm mode you just what you do is that you go here the physics and you see the electric field component solved for so for t mode just remember that always for t mode you click in plane vector and for tm mode you just click out of plane the all the analysis remains same and then you just go build all then build mesh and then you hit compute and then you will get this kind of band structure for tm that is see the back two bands meet here and there is a band gap again and then this will start okay so i hope that is clear and i hope that you will be able to simulate the photonic the photonic band gap for 2d photonic crystal structures okay So, thank you. So, this is all for the lecture on analysis and engineering of 2D photonic band structures. If you have any queries regarding any part of this lecture, you can drop an email to this particular email address. Thank you.

Thank You

